http://www.cas.org/support/stngen/stndoc/properties.html

```
=> s ibuprofen/cn
L1            1 IBUPROFEN/CN

=> d

L1   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   15687-27-1  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   Benzeneacetic acid, α-methyl-4-(2-methylpropyl)-  (CA INDEX NAME)
OTHER NAMES:
CN   (±)-α-Methyl-4-(2-methylpropyl)benzeneacetic acid
CN   (±)-2-(p-Isobutylphenyl)propionic acid
CN   (±)-Ibuprofen
CN   (±)-Ibuprophen
CN   (4-Isobutylphenyl)-α-methylacetic acid
CN   (RS)-Ibuprofen
CN   α-(4-Isobutylphenyl)propionic acid
CN   α-Methyl-4-(2-methylpropyl)benzeneacetic acid
CN   2-(4'-Isobutylphenyl)propionic acid
CN   2-(4-Isobutylphenyl)propanoic acid
CN   2-(p-Isobutylphenyl)propionic acid
CN   4-Isobutyl-α-methylphenylacetic acid
CN   4-Isobutylhydratropic acid
CN   Act 3
CN   Actiprofen
CN   Adex 200
CN   Adran
CN   Advil
CN   Alaxan
CN   Algi-Flanderil
CN   Algiflex
CN   Algofen
CN   Am-Fam 400
CN   Amibufen
CN   Anafen
CN   Anco
CN   Andran
CN   Anflagen
CN   Antarene
CN   Antiflam
CN   Apo-Ibuprofen
CN   Apsifen
CN   Artofen
CN   Artril
CN   Artril 300
CN   Atril 300
CN   Balkaprofen
CN   Betaprofen
CN   Bloom
CN   Bluton
CN   Brofen
CN   Brufanic
CN   Brufen
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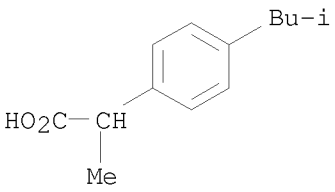
CN Brufen 400
CN Brufen Retard
CN Bruflam
CN Brufort
CN Buburone
CN Buluofen
CN Burana
CN Ibuprofen
ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT - Use FCN, FIDE, or ALL for DISPLAY
DR 58560-75-1, 139466-08-3
MF C13 H18 O2
CI COM
LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CABA, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DRUGU, EMBASE, HSDB*, IFICDB, IFIPAT, IFIUDB, IMSCOSEARCH, IMSDRUGNEWS, IMSPATENTS, IMSPRODUCT, IMSRESEARCH, IPA, MEDLINE, MRCK*, MSDS-OHS, PATDPASPC, PHAR, PIRA, PROMT, PROUSDDR, PS, RTECS*, SCISEARCH, SPECINFO, SYNTHLINE, TOXCENTER, ULIDAT, USAN, USPAT2, USPATFULL, USPATOLD, VETU
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**, WHO
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10189 REFERENCES IN FILE CA (1907 TO DATE)
295 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
10234 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	7.61	8.30

FILE 'CAPLUS' ENTERED AT 16:22:15 ON 17 APR 2008

FILE COVERS 1907 - 17 Apr 2008 VOL 148 ISS 16
FILE LAST UPDATED: 16 Apr 2008 (20080416/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

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=> s 15687-27-1/prep
         10234 15687-27-1
       4559046 PREP/RL
L2         664 15687-27-1/PREP
                 (15687-27-1 (L) PREP/RL)

=> s 15687-27-1/proc
         10234 15687-27-1
       4312272 PROC/RL
L3        1261 15687-27-1/PROC
                 (15687-27-1 (L) PROC/RL)

=> s 15687-27-1/pur
         10234 15687-27-1
        278306 PUR/RL
L4           59 15687-27-1/PUR
                 (15687-27-1 (L) PUR/RL)

=> s l2 or l3 or l4
L5         1904 L2 OR L3 OR L4

=> s l5 and palladium
        176569 PALLADIUM
L6           70 L5 AND PALLADIUM

=> s l6 and py<2003
      22929815 PY<2003
L7           52 L6 AND PY<2003

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exchange resin or zeolite)
        555617 ACTIVATED
       1356558 CARBON
         53030 ACTIVATED CARBON
                 (ACTIVATED(W)CARBON)
        569020 SILICA
        534872 GEL
         96261 SILICA GEL
                 (SILICA(W)GEL)
       1030281 ALUMINUM
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       1856565 OXIDE
        102924 ALUMINUM OXIDE
                 (ALUMINUM(W)OXIDE)
        632611 ADSOR?
       1253908 ION
        602580 EXCHANGE
        662782 RESIN
         18493 ION EXCHANGE RESIN
                 (ION(W)EXCHANGE(W)RESIN)
        106213 ZEOLITE
L8           4 L7 AND (ACTIVATED CARBON OR SILICA GEL OR ALUMINUM OXIDE OR ADSO
               R? OR ION EXCHANGE RESIN OR ZEOLITE)

=> d 1-4 ibib abs hitstr

L8   ANSWER 1 OF 4  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2002:552598  CAPLUS
DOCUMENT NUMBER:          137:249479
TITLE:                    Anchored Pd Complex in MCM-41 and MCM-48: Novel
                          Heterogeneous Catalysts for Hydrocarboxylation of Aryl
                          Olefins and Alcohols
AUTHOR(S):                Mukhopadhyay, Kausik; Sarkar, Bibhas R.; Chaudhari,
                          Raghunath V.
CORPORATE SOURCE:         Homogeneous Catalysis Division, National Chemical
                          Laboratory, Pune, 411008, India
SOURCE:                   Journal of the American Chemical Society (2002
                          ), 124(33), 9692-9693
                          CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER:                American Chemical Society
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
AB   Synthesis of anchored Pd complexes in mesoporous supports such as MCM-41
     and MCM-48 as true heterogeneous catalysts for hydrocarboxylation of aryl
     olefins and alcs. to give excellent conversion (.apprx.100%) and
     regioselectivity (.apprx.99%) for 2-arylpropionic acids.  The catalysts
     were characterized by powder-XRD, 31P CP-MAS NMR, FT-IR, TEM, XPS and
     ICP-AES.  Recycle studies with these anchored Pd mesoporous catalysts were
     performed to confirm true heterogeneity.
IT   15687-27-1P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (hydrocarboxylation of aryl olefins and alcs. catalyzed by anchored Pd
        complexes in mesoporous supports such as MCM-41 and MCM-48)
RN   15687-27-1  CAPLUS
CN   Benzeneacetic acid, α-methyl-4-(2-methylpropyl)-  (CA INDEX NAME)
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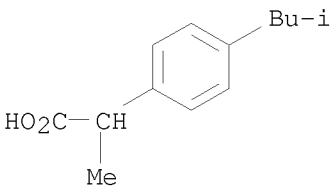


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REFERENCE COUNT:          24    THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS
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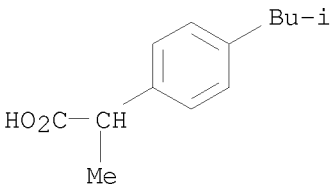
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:228466 CAPLUS
DOCUMENT NUMBER: 128:309668
TITLE: Catalytic carbonylation for the synthesis of chemical intermediates
AUTHOR(S): Kim, Young Gul; Lee, Jae Sung; Lee, Kyung Hee
CORPORATE SOURCE: Department of Chemical Engineering and School of Environmental Engineering, Pohang Univ. of Science and Technology, Pohang, 790-784, S. Korea
SOURCE: Research on Chemical Intermediates (1998), 24(2), 197-211
CODEN: RCINEE; ISSN: 0922-6168
PUBLISHER: VSP BV
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Chemical related to three catalytic carbonylation reactions is discussed. Synthesis of diphenylurea from nitrobenzene, aniline, and CO gives isolated yields above 98% at 100°-120° and 15-60 bar of CO in the presence of a palladium(II) complex, PPh3 and NEt4Cl. Exptl. evidence was provided to prove a new reaction stoichiometry and involvement of a carbamoyl intermediate. In carbonylation of HCHO over ion exchange resin catalysts, reaction temperature, time, pressure, and solvent were important variables to obtain high yields of Me glycolate. Carbonylation of isobutylphenylethanol at 120° and 40 bar of CO in the presence of PdCl2-PPh3-HCl gives 98% yield of α-(4-isobutylphenyl) propionic acid (ibuprofen). Each catalyst component had a definite role that is indispensable for an efficient overall reaction.
IT 15687-27-1P, α-(4-Isobutylphenyl)propionic acid
RL: IMF (Industrial manufacture); PREP (Preparation)
(catalytic hydrocarbonylation for synthesis of isobutylphenyl propionic acid)
RN 15687-27-1 CAPLUS
CN Benzeneacetic acid, α-methyl-4-(2-methylpropyl)- (CA INDEX NAME)



REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:228540 CAPLUS
DOCUMENT NUMBER: 114:228540
TITLE: Preparation of alpha-(4-isobutylphenyl)propionic acid and its precursors alpha-(4-isobutylphenyl)propionaldehyde and methyl

alpha-(4-isobutylphenyl)propionate from isobutylbenzene

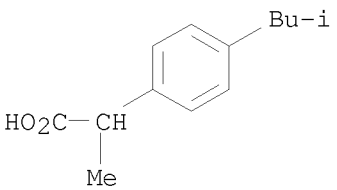
INVENTOR(S): Tokumoto, Yuuichi; Shimizu, Isoo; Inoue, Satoru
PATENT ASSIGNEE(S): Nippon Petrochemicals Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 39 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 414207	A2	19910227	EP 1990-115995	19900821 <--
EP 414207	A3	19911023		
EP 414207	B1	19940803		
R: CH, DE, FR, GB, IT, LI, SE				
JP 03083948	A	19910409	JP 1989-220009	19890825 <--
CA 2023679	A1	19910226	CA 1990-2023679	19900821 <--
CA 2023679	C	19980818		
US 5166419	A	19921124	US 1990-571178	19900822 <--
KR 187301	B1	19990515	KR 1990-13301	19900825 <--
JP 10182541	A	19980707	JP 1998-12856	19980126 <--
JP 2851276	B2	19990127		

PRIORITY APPLN. INFO.: JP 1989-220009 A 19890825
OTHER SOURCE(S): CASREACT 114:228540; MARPAT 114:228540
AB A method for preparing α-(4-isobutylphenyl)propionic acid (I) or its precursors Me α-(4-isobutylphenyl)propionate (II) or α-(4-isobutylphenyl)propionaldehyde (III) at low cost and high purity is claimed. I is a useful medicine (Code name ibuprophen). The method for the preparation of I-III comprises 3 steps: a) subjecting isobutylbenzene and a polyalkylbenzene to disproportionation reaction to form p-isobutyl(ethyl)benzene b) dehydrogenating p-isobutylethylbenzene to form p-isobutylstyrene and c) hydrocarboxylation, hydroesterification, or hydroformylation of p-isobutylstyrene to give I-III resp. Thus, disproportionation reaction of isobutylbenzenes with diethylbenzene in the presence of HY zeolite catalyst gave p-isobutylethylbenzene (64.1 weight % conversion and 46.3 mol % selectivity). Dehydrogenation of p-isobutylethylbenzene with iron oxide catalyst containing K and Cr as promoters gave p-isobutylstyrene with 83% selectivity and 31% conversion. Standard conversion procedures of p-isobutylstyrene were applied to give the desired compds. I-III.

IT 15687-27-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 15687-27-1 CAPLUS
CN Benzeneacetic acid, α-methyl-4-(2-methylpropyl)- (CA INDEX NAME)



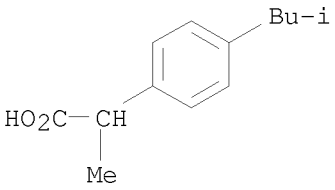
L8 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:611548 CAPLUS
DOCUMENT NUMBER: 113:211548
ORIGINAL REFERENCE NO.: 113:35735a,35738a
TITLE: Preparation of p-isobutylstyrene as an ibuprofen intermediate
INVENTOR(S): Shimizu, Isoo; Matsumura, Yasuo; Tokumoto, Yuichi; Uchida, Kazumichi
PATENT ASSIGNEE(S): Nippon Petrochemicals Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 19 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 373362	A1	19900620	EP 1989-120734	19891108 <--
EP 373362	B1	19930203		
R: CH, DE, FR, GB, IT, LI, SE				
JP 02256627	A	19901017	JP 1989-149125	19890612 <--
JP 2756828	B2	19980525		
JP 02256629	A	19901017	JP 1989-149126	19890612 <--
JP 2756829	B2	19980525		
CA 2002243	A1	19900613	CA 1989-2002243	19891106 <--
CA 2002243	C	19971230		
US 5436402	A	19950725	US 1994-323600	19941017 <--

PRIORITY APPLN. INFO.:

JP 1988-314153	A	19881213
US 1989-435776	B1	19891113
US 1992-917799	B1	19920720
US 1993-62703	B1	19930514

AB Claimed is a method for preparing pure p-isobutylstyrene. The said method comprises reacting o- and/or m-isobutylethylbenzene, optionally, together with isobutylbenzene in the presence of an acid catalyst at a reaction temperature of -10 to 600° so that the production of sec-butylethylbenzene (I) does not exceed 20% by weight Dehydrogenation of the resulting mixture of p-isobutylethylbenzene and I in the presence of a dehydrogenation catalyst containing at least one metal from groups Ib, IIb, VIa, VIIa, and VIII of the periodic table gives p-isobutylstyrene. A mixture containing isobutylbenzene (II) 81.8, o-isobutylethylbenzene (III) 7.5, m-isobutylethylbenzene (IV) 5.5, p-isobutylethylbenzene (V) 1.2 weight % was treated with CF_3SO_3H at 110° for 24 h to give II 78.7, III 3.1, IV 7.3, and V 4.7 weight %. Dehydrogenation of V gave p-isobutylstyrene.
IT 15687-27-1P, α-(4-Isobutylphenylpropionic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, method for)
RN 15687-27-1 CAPLUS
CN Benzeneacetic acid, α-methyl-4-(2-methylpropyl)- (CA INDEX NAME)


Bu-i
HO2C
CH
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